

Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-  
1546-95-8 | DTXSID70165670

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.48 days

Global applicability domain: Outside

Local applicability domain index: 2.67e-01

Confidence level: 7.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tetradeca-1,13-diene</div> <div>Measured: 367</div> <div>Predicted: 8.69</div>	<div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 12.5</div> <div>Predicted: 3.99</div>	<div>Image not found</div> <div>2-Methylhexane</div> <div>Measured: 12.5</div> <div>Predicted: 5.54</div>
<div>Image not found</div> <div>2-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 4.23</div>		